From Raw Physical Data to Reliable Thermodynamic Model Parameters

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Nowadays actual process simulation packages are reliable and valuable tools for many tasks occurring in the day of a chemical process engineer. However, the accuracy of a process simulation depends strongly on the thermodynamic models used to describe the physical behavior of the involved components. To achieve real world behavior with a model therefore one needs both reliable property data as well as a full featured data regression package. One example for a valuable source of data is the numerical database DETHERM. It contains thermophysical property data for the design and optimization of chemical plants. At the time more than 4.2 million data sets for more than 122,000 pure components and mixtures are stored. The data are collected and updated by well-known research groups, e.g. the Universities of Oldenburg and Regensburg, the DDBST and the FIZ CHEMIE. The properties stored include mainly phase equilibrium data (VLE, LLE, SLE, VLLE), vapor pressures, critical data, thermodynamic properties, transport properties, surface tensions and electrolyte data. Following up to database retrieval the DECHEMA Data Preparation Package will be used to close the gap between raw thermophysical data and model parameters, as used in any process simulation package. Retrieved or otherwise generated data sets can be displayed, compared and selected. Afterwards parameters for pure component as well as binary models can regressed and displayed in comparison with the data. The regression module is capable to correlate simultaneously different data types using different error functions. For example the simultaneous correlation of VLE, LLE, HE, gamma, gamma-infinity and azeotropic data is possible. The package is not restricted to its built-in thermodynamic models. Thermodynamic calculations are performed using a standardized interface. This enables users to simply plug in any thermodynamic package and/or model of their own choice.